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ABSTRACT

The outstanding properties of carbon nanotubes (CNTs) keep attracting the attention of researchers from different fields. CNTs are promising candidates for applications e.g. in lightweight construction but also in electronics, medicine and many more. The basis for the realization of the manifold applications is a detailed knowledge of the material properties of the carbon nanotubes. In particular for applications in lightweight constructions or in composites, the knowledge of the mechanical behavior of the CNTs is of vital interest. Hence, a lot of effort is put into the experimental and theoretical determination of the mechanical material properties of CNTs. Due to their small size, special techniques have to be applied. In this research, a modified molecular structural mechanics model for the numerical determination of the mechanical behavior of carbon nanotubes is presented. It uses an advanced approach for the geometrical representation of the CNT structure while the covalent bonds in the CNTs are represented by beam elements. Furthermore, the model is specifically designed to overcome major drawbacks in existing molecular structural mechanics models. This includes energetic consistency with the underlying chemical force field. The model is developed further to enable the application of a more advanced chemical force field representation. The developed model is able to predict, inter alia, the lateral and radial stiffness properties of the CNTs. The results for the lateral stiffness are given and discussed in order to emphasize the progress made with the presented approach.

Keywords: Carbon Nanotubes, CNT, Molecular Mechanics, Molecular Structural Mechanics, nano, mechanical properties

1. INTRODUCTION

Carbon nanotubes (CNTs) are nanoscopic structures made of carbon atoms arranged in a hexagonal manner. Due to the hexagonal structure, each carbon atom is surrounded by three neighboring carbon atoms. The bond of a carbon atom to each of its three neighbors is a sp^2-hybridized covalent bond. This is also typical for graphene which is closely related to carbon nanotubes. As a result of this, one can also imagine the carbon nanotube as a cut-out of a graphene sheet which is then rolled up into a seamless tube. The size and the cutting direction of such a cut-out determines the diameter, length and type of the single wall carbon nanotube. Regarding the type of the carbon nanotube one needs to distinguish between so called multi wall carbon nanotubes and single wall carbon nanotubes. As the name already suggests, the single wall carbon nanotubes are made out of a single layer of carbon, while the multi wall carbon nanotubes are basically several single wall carbon nanotubes stacked together sharing a common center axis. The single wall carbon nanotubes can then be further distinguished into three types which are called *armchair*, *zig-zag* or *chiral*. The SWCNT types are characterized by different unit cells which can be defined by using a so called index pair (n, m). The index pair describes the chirality vector $\vec{C}$ in terms of the graphene basis $\vec{a}_1$ and $\vec{a}_2$, see figure 1. Here, the chirality vector defines one edge where the graphene sheet needs to be cut in order to construct the unit cell of the desired carbon nanotube. Perpendicular to the chirality vector, the translational vector $\vec{T}$, which can be calculated based on the index pair (n, m) defines the second cutting edge. Since the numbers in the index pair have to be natural numbers, the graphene cut-out

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defining the carbon nanotube can not be constructed in arbitrary limits. As a result, only discrete values for the nanotube diameter depending on the nanotube type can be obtained. The type of the constructed nanotube can be recognized on the basis of the index pair (n, m), where (n, n) depicts armchair carbon nanotubes, $(n, 0)$ zig-zag carbon nanotubes and (n, m) (with $n > m$, $m \neq 0$) chiral carbon nanotubes.

The reasons why carbon nanotubes are such an interesting material, in particular with respect to their mechanical properties, are manifold. During the last two decades of carbon nanotube research a multitude of different applications were proposed from very different fields ranging e.g. from medicine and electronics to applications in lightweight construction. It can be shown by the specific example of novel carbon fibers spun out of carbon nanotubes, that carbon nanotubes are a promising material due to to their outstanding mechanical properties, e.g. see Le et al.[1] These fibers were proposed as a possible successor for state of the art carbon fibers. In order to push these fibers towards application, the knowledge of their specific properties is vital. This includes (i) knowledge of the material properties, in particular the elastic properties, of the individual carbon nanotubes *within* the fiber as well as (ii) knowledge of the interactions happening *between* the individual carbon nanotubes. The present research deals with the first aspect of this, the second one was partly covered in Eberhardt and Wallmersperger.[2]

The knowledge of the mechanical behavior of carbon nanotubes is, in principle, accessible via experimental investigations. However, due to the small scale (atomic scale) of the carbon nanotubes it is a big challenge to design and conduct tests able to determine, e.g. the elastic properties of an individual single wall carbon nanotube. As a result of this, the obtained results suffer from large error bars. Hence, theoretical models of the carbon nanotubes and their related (numerical) simulations play an even more important role for the illumination of the unknown material properties of carbon nanotubes. As the seemingly most natural approach to tackle problems on the atomistic scale, usually quantum mechanical approaches based on the solution of the Schrödingerequation first come to the mind. However, to enable the calculation of results in the first place, it is necessary to introduce a multitude of assumptions and simplifications and even then, the feasible system size which can be addressed with reasonable computational effort is limited. As a classical mechanics alternative, the so called molecular mechanics methods were established which are based on the application of chemical force fields. This kind of method goes along with a strongly reduced computational effort while maintaining sufficient accuracy for the obtained results. As a result of these considerations, we have chosen an approach from the class of molecular mechanics to address the scientific problems in the present research.

The paper is structured as follows. At first the most relevant literature contributions of the field are mentioned in section 2 to give the current state of the art. In section 3, the so called Molecular Structural Mechanics model is briefly introduced, and some limitations of the model in its current state are identified. Subsequently, a way to overcome these drawbacks is developed. The key idea is here to implement a more sophisticated chemical force field. After this implementation is done, key results of the model are given in section 4 and compared to results obtained with the original model without the proposed modifications.

2. LITERATURE REVIEW

Due to their promising properties for possible applications in many fields, carbon nanotubes have received great attention from researchers all over the world during the last two decades resulting in a vast amount of scientific contributions. In the present short literature review only the most relevant works regarding the determination of the elastic properties of single wall carbon nanotubes based on molecular mechanics methods shall be mentioned in a concise manor. For the interested reader who wants to get a more extensive overview on the efforts made with respect to the modeling of single wall carbon nanotubes, the authors recommend the reviews given by Rafiee and Moghadam[3] as well as Sakharova et al.[4]

The mechanical modeling of single wall carbon nanotubes has been approached with the help of a multitude of theories ranging from quantum-mechanical approaches in different varieties, given e.g. by Sánchez-Portal et al.,[5] Chandraseker and Mukherjee[6] and Domínguez-Rodríguez et al.,[7] up to methods based on classical continuum mechanics, e.g. research done by Odegard et al.[8] or Cinefra at al.[9] A classical approach trying to take into account the discrete nature of the carbon nanotubes can be found within the framework of so called molecular mechanics. Here, covalent bonds within the carbon nanotube are represented by structural elements like for instance spring elements, or, like it is applied in the present work, by beam elements. Models using spring elements for the representation of the covalent bonds were developed e.g. by Meo and Rossi[10] as well as by

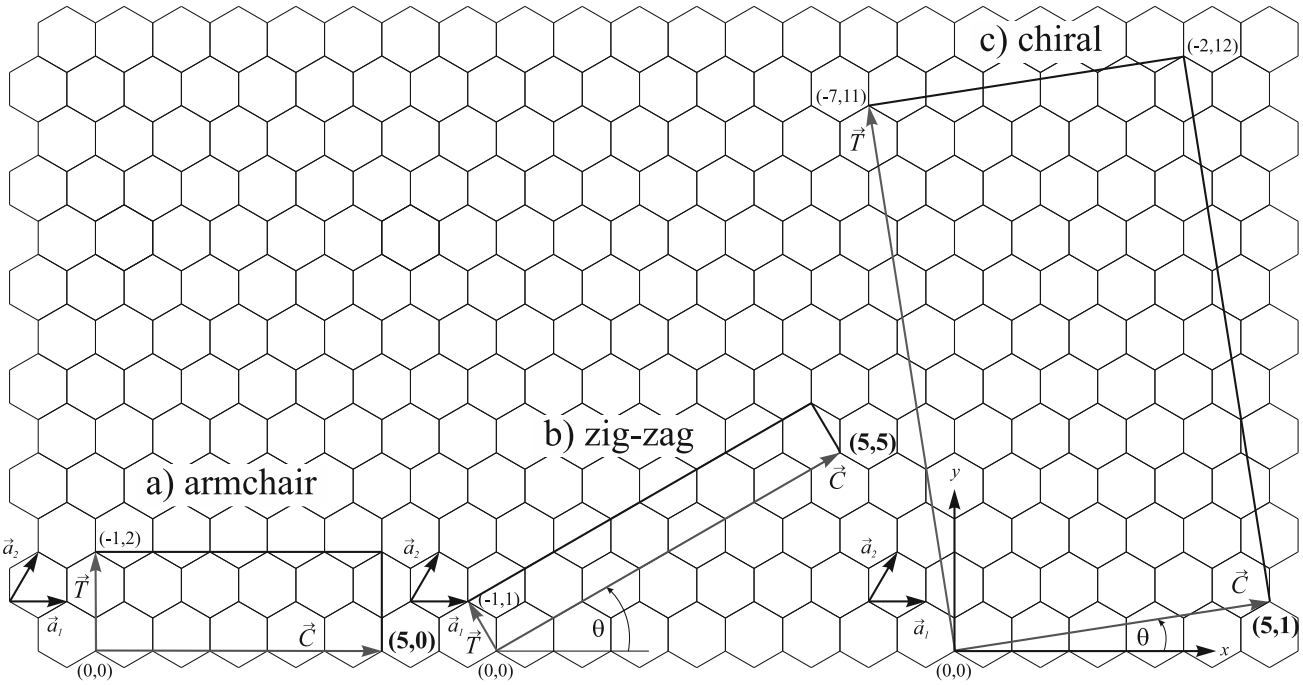


Figure 1. Unit cell construction for the three single wall carbon nanotube types.

Giannopoulos et al.[11 12] The idea to apply beams to model the covalent bonds was first proposed by Li and Chou[13] who also introduced the name "Molecular Structural Mechanics" (MSM) for this type of molecular mechanical carbon nanotube model. The applicability of the MSM model in particular with respect to its implementation in Finite-Element codes was improved by Tserpes and Papanikos.[14] Extensions of the model to improve its ability to predict radial stiffness properties were made by Chen et al.[15] who proposed to introduce a beam with an cross-section exhibiting different principal axial moments of inertia. Eberhardt and Wallmersperger investigated - on the basis of the MSM model - the deformation behavior of single wall carbon nanotubes under tension.[16] The original work of Li and Chou[13] was also used during the years by a vast number of, researchers which reproduced their results for the elastic properties of single wall carbon nanotubes. The MSM model was developed into a modified MSM model by Eberhardt and Wallmersperger[17] who found, that the original model is not consistent with its underlying chemical force field in terms of energy. A newly developed approach to take the bond angle changes in the carbon nanotubes into account was introduced into the MSM model which resolved this problem and created an energy consistent MSM model. On the basis of this model, Xia et al.[18] created a model for the determination of the wrinkling behavior of annular graphene sheets and its elastic properties. All the works related to the MSM method mentioned so far rely on harmonic potentials regarding their underlying chemical force field representations.

3. MODELING

3.1 Molecular Structural Mechanics Approach for the determination of elastic properties of single wall carbon nanotubes

In the molecular mechanics approaches, the interactions of the incorporated atoms, realized by chemical bonds, are usually considered by applying a chemical force field. In the specific molecular mechanics model chosen in the present research, the key idea is, that the bond between the carbon atoms can be described with the help of truss-beam-twist elements. For convenience, from now on they will be referred to simply as beam elements. This approach is called the Molecular Structural Mechanics (MSM) model. By incorporating the beam elements as a mechanical replacement for the chemical (covalent) bonds, it is necessary to transfer the chemical properties

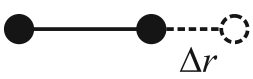
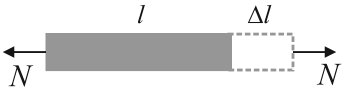
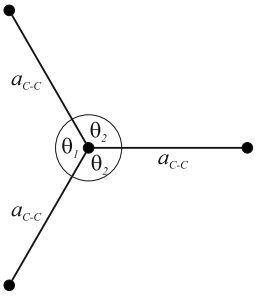
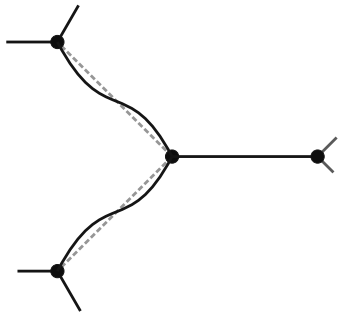
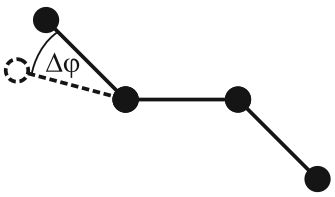
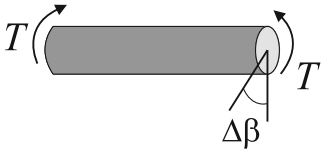
bond deformations	**resulting equations**	**beam deformations**
bond stretching 	$k_r = \frac{EA}{l}$	beam stretching 
$U_r = \frac{1}{2}\, k_r\, \Delta r^2$		$U_N = \frac{1}{2}\frac{EA}{l}\Delta l^2$
bond angle bending 	$k_\theta = 2\,\frac{EI}{l}$	beam bending 
$U_\theta = \frac{3}{4}\, k_\theta \Delta\theta_1^2$		$U_M = \frac{3\,E\pi d^4}{128\,l}\Delta\theta_1^2$
bond twisting 	$k_\tau = \frac{GJ}{l}$	beam twisting 
$U_\tau = \frac{1}{2}\, k_\tau\, \Delta\phi^2$		$U_T = \frac{1}{2}\frac{GJ}{l}\Delta\beta^2$

Figure 2. Overview over the MSM approach developed in Eberhardt and Wallmersperger.[17]

described on the basis of the chemical force field to the mechanical beams. This means, that the parameters mandatory to define the beam elements - like their material properties and geometrical dimensions - have to be calculated based on information given by the chemical force field. In the most simplest case, the chemical force field is in turn characterized by a set of constants k, the so called chemical force constants. Beside the representation of the covalent bonds, the correct consideration of the geometry of the carbon nanotube is also of importance. This will not be discussed in detail in the present paper. The interested reader is referred to previous works given by Eberhardt and Wallmersperger[16].[17]

The original paper of the development of the MSM model was published by Li and Chou.[13] The here proposed model is based on their work, however strongly modified.[17] The basic idea and starting point of the model is to examine at first the possible bond deformations occurring in the bonds of the carbon nanotube, see figure 2. These are the stretching of the bond, the change of the bond angle between two bonds and the torsion of a bond. Since in the present MSM model structural elements are chosen to represent the covalent bonds, the structural elements are chosen in that way, that they can mimic the bond deformations. The chosen beam element is capable of fulfilling this condition since the beam can stretch, bend and twist. This is given in the last column of figure 2. In order to calculate the mandatory beam parameters in a way where they fit the behavior of the carbon nanotube governed by the chemical force field, it is necessary to create a connection between the mechanical domain of the beams and the chemical domain of the chemical force field. In order to obtain this connection, the governing potentials are formulated. In the chemical domain, these potentials are given by the chosen chemical force field. In the most simple case, like e.g. in Li and Chou,[13] the total potential is calculated from three contributing harmonic potentials, see figure 2. Harmonic means, that the order of the potential function is quadratic and the potential is characterized by a corresponding chemical force constant k_i. As a result, the total chemical potential is the sum of all contributing harmonic potentials:

$$U_{total}^{harmonic} = \frac{1}{2}\, k_r\, \Delta r^2 + \frac{1}{2}\, k_\theta\, \Delta\theta^2 + \frac{1}{2}\, k_\tau\, \Delta\varphi^2. \tag{1}$$

In the mechanical domain, the potential describing the deformations of the beam are given by the strain energies. When a linear-elastic material is assumed, the resulting linear-elastic strain energies are given in figure 2. By comparing the corresponding energies in beams and bonds for the same deformations one can state the equivalence between the energy contributions, This results in a set of three equations depicted in figure 2. For details in the derivation of the equations, the interested reader is referred to Eberhardt and Wallmersperger.[17] This set of three equations enables the calculation of the mandatory beam parameters from the information given by the chemical force fields. The beam parameters are determined by simply solving the equations which leads to the following expressions for the local Young's modulus E, shear modulus G and beam diameter d (a circular cross-section is assumed) of a single beam:

$$E = \frac{k_r^2\, L}{2\pi k_\theta} \tag{2}$$

$$G = \frac{k_\tau\, L\, k_r^2}{2\pi k_\theta^2} \tag{3}$$

$$d = \frac{4}{\sqrt{2}} \sqrt{\frac{k_\theta}{k_r}} \tag{4}$$

The equations given above establish the desired connection between the chemical force field description and the mechanical parameters of one single beam. After the beam properties are calculated by the given approach, it is possible to create the beam representation of the carbon nanotube by placing beam elements in accordance with the desired carbon nanotube geometry. In the present research, the beam representation was implemented in the commercial Finite-Element tool ABAQUS by using the provided native beam elements from the elements library of ABAQUS. The tube modulus calculated by this model is given in section 4 of the present paper.

3.2 Integration of the 2nd generation Reactive Bond Order Potential in the Molecular Structural Mechanics model

The foundation of the proposed MSM model is the chemical potential. As already stated, the potential so far applied is of the most simple type since it is based on harmonic functions. The application of these simple

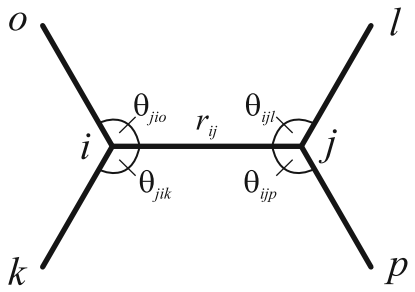


Figure 3. Covalent bond between the atoms i and j and their next neighbors k, l, o and p including bond angles θ and bond length r_{ij}.

potentials comes with several limitations also affecting the applicability of the MSM model. Shortcomings stemming from the use of harmonic potentials are, inter alia:

- The potential is independent on the environment of the considered bond.
- The potential only depends on changes of the bond geometry (stretching, bending, twisting) but not on the total value of e.g. the bond angle between two bonds.
- The harmonic potentials are only applicable with reasonable accuracy for small deformations of the bond.

This leads to the question whether the harmonic potentials deliver valid results or just coarse approximations. This question is best answered by implementing a sophisticated chemical potential followed by an investigation of the obtained results. In the present research, the 2nd generation reactive bond order potential (REBO) developed by Brenner and co-workers[19] was implemented. The limitations of the harmonic potential, as given above, are not present in the 2nd generation REBO potential. For instance, the potential is able to take the environment of the bond into account. Since the 2nd generation REBO potential is a force field which considers the nearest neighbors of the atoms, it includes the influence on the adjacent atoms or bonds respectively. It also includes total values, e.g. for the bond angle, instead of only changes in the deformation values. Furthermore, the 2nd generation REBO potential is also applicable beyond the small deformations regime up to bond breaking. The total potential surface based on the 2nd generation REBO potential is calculated as follows:

$$U_{total}^{REBO} = \sum_{i} \sum_{j>i} \left[V^R\left(r_{ij}\right) - b_{ij} V^A\left(r_{ij}\right) \right]. \tag{5}$$

This means, that the total potential surface U_{total}^{REBO} is the sum over all bonds between the atoms i and j in the considered structure, here applied to carbon nanotubes. In addition to this, also the direct neighbors to the atoms i and j are taken into account. They are marked with the indices k, l, o and p. Hence, the fundamental structure considered for the calculation of a single bond contribution for the total potential is the one depicted in figure 3. The expressions $V^R(r_{ij})$ and $V^A(r_{ij})$ in equation (5) represent the repulsive and attractive contributions of the bond depending on the distance between the two atoms i and j and hence the bond length. The parameter b_{ij} includes the effects of the bond angles θ as well as the twist τ of the bond. The above mentioned expressions are characterized by a larger set of parameters compared to only three parameters (k_τ, k_θ, k_τ) needed to characterize the harmonic potential. Nevertheless, the same bond deformations already considered to be present in the original MSM approach, see also figure 2, are present in the 2nd generation REBO potential. Further details of the mentioned expressions are given in Brenner at al.[19]

When it comes to the implementation of the new potential into the existing framework of the MSM method, some differences have to be taken into account compared to the original approach. In the MSM model using the harmonic potentials, see section 3.1, the contributions of the different deformations given in figure 2 were strictly separated, see equation (1). As a result of this, the chemical force constants k_i could be directly applied to calculate the beam parameters E, G and d. When using the 2nd generation REBO potential, the contributions of the different deformations are part of a mixed formulation in the total potential, see equation (5). Since there

are no chemical force constants available to be used in equations (2) - (4), some modifications to the original MSM approach have to be done. The fundamental idea for the modification is, that it would be desirable to use the existing MSM framework to the largest possible extent. This goal can be achieved by a new step introduced into the existing framework which targets at the calculation of *artificial* chemical force constants (k_r^{ij}, k_θ^{ij}, k_τ^{ij}) on the basis of the total potential energy. These are calculated as derivatives of the total potential with respect to the deformation values:

$$k_r^{ij} = \frac{\partial^2 U_{total}^{REBO}}{\partial r_{ij}^2} \tag{6}$$

$$k_\theta^{ij} = \frac{\partial^2 U_{total}^{REBO}}{\partial \theta_{jik}^2} + \frac{\partial^2 U_{total}^{REBO}}{\partial \theta_{j'i'k'}^2} + \frac{\partial^2 U_{total}^{REBO}}{\partial \theta_{k''i''o''}^2} \tag{7}$$

$$k_\tau^{ij} = \frac{\partial^2 U_{total}^{REBO}}{\partial \tau_{ijkl}^2} + \frac{\partial^2 U_{total}^{REBO}}{\partial \tau_{ijkp}^2} + \frac{\partial^2 U_{total}^{REBO}}{\partial \tau_{ijol}^2} + \frac{\partial^2 U_{total}^{REBO}}{\partial \tau_{ijop}^2}. \tag{8}$$

The indices in the equations point out the atoms participating in the corresponding bond length, bond angle or bond twist respectively. While k_r^{ij} only consist of a single expression, the force constants k_θ^{ij} and k_τ^{ij} have to be assembled out of several contributions. The indices marked with one or two primes in equation (7) depict that a single bond angle is part of three bond systems, e.g. jik, $j'i'k'$, and $k''i''o''$. The upper indices ij in the artificial force constants depict, in contrast to the MSM model using harmonic potentials, that now *bond-specific* force constants are used for the bond between the atoms i and j. The artificial force constants enable the calculation of, now likewise *bond-specific*, beam parameters E_{ij}, G_{ij} and d_{ij}. Together with the proper consideration of the carbon nanotube geometry the beam framework representing the carbon nanotube can be created and used to conduct e.g. a virtual tensile test and obtain results for the elastic properties which are discussed in the next section.

4. RESULTS

The results given in the present research are obtained from a virtual tensile test carried out with a selection of armchair and zig-zag single wall carbon nanotubes. To conduct this virtual tensile test, the investigated tube is fixed at one end, while the other end remains free but is subjected to a tensile force distributed along the atoms at the edge of the carbon nanotube.

The virtual tensile test aims at obtaining elastic properties of the carbon nanotube. In particular, the literature usually deals here with the calculation of a property which is often referred to as "Young's modulus" of the carbon nanotube. As a matter of fact this property is usually calculated in an analogous manner like the Young's modulus e.g. of a steel rod subjected to a real tensile test. However, a carbon nanotube is a structure on the atomistic level and hence not a continuous material like the mentioned steel. As a result of this, it is the authors opinion, that "Young's modulus" is an unfortunate expression for the here determined elastic property. Here, this drawback is avoided by simply using a different notion. In the present paper, the elastic property usually referred to as "Young's modulus" is called "tube modulus". However, this measure is calculated analogously like the Young's modulus of a macroscopic specimen on the basis of the known tensile force and the resulting tip displacement of the carbon nanotube. In the present research, we investigated the tube modulus for armchair and zig-zag carbon nanotubes in a diameter range of 2 Å to 17 Å. The results obtained by applying the MSM model with (i) a harmonic force field representation (see section 3.1) and (ii) a 2nd generation reactive bond order potential (see section 3.2) are given in figure 4.

The results obtained for the tube modulus based on the harmonic potentials approach show for both, armchair and zig-zag single wall carbon nanotubes, that the tube modulus monotonically increases with increasing nanotube diameter, see figure 4. In general, the tube modulus of the zig-zag carbon nanotubes is smaller than the one of the armchair carbon nanotubes. However, the difference decreases for increasing nanotube diameters as the value for the tube modulus converges to approximately 800 GPa.

The results obtained by using the sophisticated 2nd generation REBO potential show a different trend: Carbon nanotubes with smaller diameters show a remarkable higher tube modulus than larger diameter nanotubes, see figure 4. The virtual tensile test conducted with the smallest investigated armchair carbon nanotube yields a tube

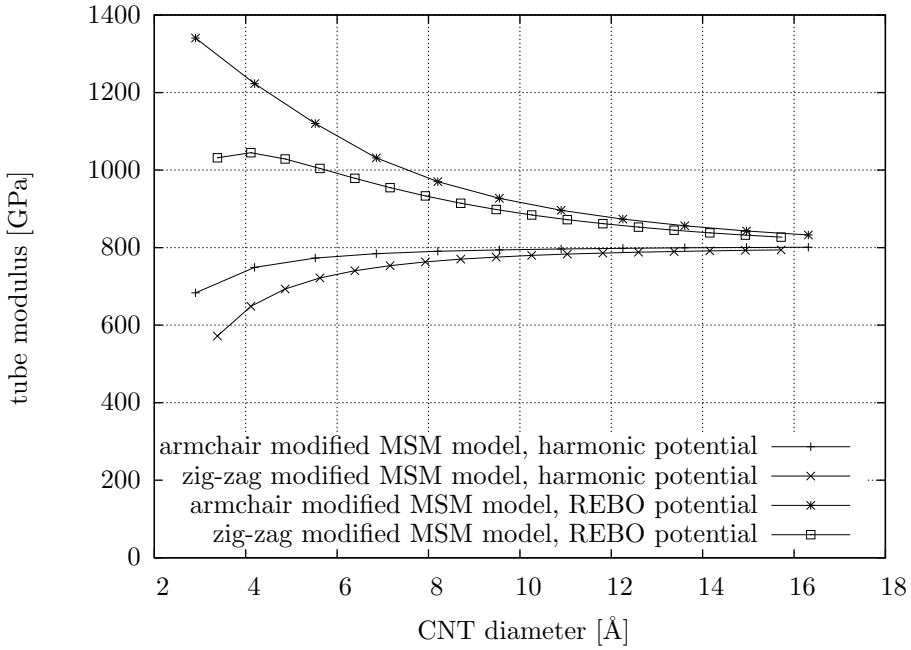


Figure 4. Resulting tube modulus for armchair and zig-zag single wall carbon nanotubes using the modified MSM model according to Eberhardt and Wallmersperger.[17]

modulus of approximately 1350 GPa. With increasing nanotube diameters, the tube modulus of the armchair as well as the zig-zag carbon nanotubes decreases to approx. 830 GPa for the largest investigated nanotubes. The trend of the curves seem to reach a convergent value in this area. Again, the tube modulus obtained for the zig-zag carbon nanotubes is in general smaller than the one calculated for the armchair nanotubes.
Comparing the results gained with the harmonic potentials with those obtained with the 2nd generation REBO potential one can state, that the results are very different in terms of the evolution of the tube modulus with respect to the diameter. However, with increasing nanotube diameters both approaches converge at approximately 800 GPa.

5. CONCLUSION AND OUTLOOK

In the present research a modified molecular structural mechanics (MSM) model for the determination of the elastic properties of single wall carbon nanotubes was proposed. Structural beam elements were used to represent the covalent bonds in the carbon nanotube. The mandatory beam parameters were calculated from the information given by the underlying chemical force field. In order to improve the accuracy and versatility of the MSM model, the simple harmonic potential approach was substituted by the sophisticated 2nd generation reactive bond order potential according to Brenner an co-workers.[19]
In section 3.2 the question was posed whether the harmonic potential is in general a suitable choice for the underlying chemical force field of the MSM model. The results given in section 4 show, that for carbon nanotubes with smaller diameters the more sophisticated 2nd generation REBO potential yields substantially different results leading to the insight, that the harmonic potentials are no good choice for the determination of the elastic properties of small diameter carbon nanotubes. However, for tubes with comparatively large diameters, the results for both chemical force fields show only a small difference and hence the application of the more simple harmonic force field seems to be admissible.
In future research, we will utilize the 2nd generation REBO force field in its full potential, e.g. when involving large deformations of the bond for the determination of the carbon nanotubes strength.

ACKNOWLEDGMENTS

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REFERENCES

[1] Lu, X. and Hu, Z., "Mechanical property evaluation of single-walled carbon nanotubes by finite element modeling," *Composites Part B: Engineering* **43**(4), 1902–1913 (2012).

[2] Eberhardt, O. and Wallmersperger, T., "Molecular mechanics methods for individual carbon nanotubes and nanotube assemblies," in [*SPIE Smart Structures and Materials+ Nondestructive Evaluation and Health Monitoring*], 94320G–94320G, International Society for Optics and Photonics (2015).

[3] Rafiee, R. and Moghadam, R. M., "On the modeling of carbon nanotubes: A critical review," *Composites Part B: Engineering* **56**, 435–449 (2014).

[4] Sakharova, N. A., Antunes, J. M., Pereira, A. F. G., and Fernandes, J. V., "Developments in the evaluation of elastic properties of carbon nanotubes and their heterojunctions by numerical simulation," *AIMS Materials Science* **4(3)** (2017).

[5] Sánchez-Portal, D., Artacho, E., Soler, J. M., Rubio, A., and Ordejón, P., "Ab initio structural, elastic, and vibrational properties of carbon nanotubes," *Phys. Rev. B* **59**, 12678–12688 (May 1999).

[6] Chandraseker, K. and Mukherjee, S., "Atomistic-continuum and ab initio estimation of the elastic moduli of single-walled carbon nanotubes," *Computational Materials Science* **40**(1), 147 – 158 (2007).

[7] Domínguez-Rodríguez, G., Tapia, A., and Avilés, F., "An assessment of finite element analysis to predict the elastic modulus and poissons ratio of singlewall carbon nanotubes," *Computational Materials Science* **82**, 257–263 (2014).

[8] Odegard, G. M., Gates, T. S., Nicholson, L. M., and Wise, K. E., "Equivalent-continuum modeling of nano-structured materials," *Composites Science and Technology* **62**, 18691880 (2002).

[9] Cinefra, M., Carrera, E., and Brischetto, S., "Refined shell models for the vibration analysis of multiwalled carbon nanotubes," *Mechanics of Advanced Materials and Structures* **18**(7), 476–483 (2011).

[10] Meo, M. and Rossi, M., "Prediction of youngs modulus of single wall carbon nanotubes by molecular-mechanics based finite element modelling," *Composites Science and Technology* **66**, 15971605 (2006).

[11] Giannopoulos, G., Kakavas, P., and Anifantis, N., "Evaluation of the effective mechanical properties of single walled carbon nanotubes using a spring based finite element approach," *Computational Materials Science* **41**(4), 561 – 569 (2008).

[12] Giannopoulos, G., Liosatos, I., and Moukanidis, A., "Parametric study of elastic mechanical properties of graphene nanoribbons by a new structural mechanics approach," *Physica E: Low-dimensional Systems and Nanostructures* **44**(1), 124 – 134 (2011).

[13] Li, C. and Chou, T.-W., "A structural mechanics approach for the analysis of carbon nanotubes," *International Journal of Solids and Structures* **40**, 24872499 (2003).

[14] Tserpes, K. and Papanikos, P., "Finite element modeling of single-walled carbon nanotubes," *Composites: Part B* **36**, 468477 (2005).

[15] Chen, W.-H., Cheng, H.-C., and Liu, Y.-L., "Radial mechanical properties of single-walled carbon nanotubes using modified molecular structure mechanics," *Computational Materials Science* **47**, 985993 (2010).

[16] Eberhardt, O. and Wallmersperger, T., "Mechanical properties and deformation behavior of carbon nanotubes calculated by a molecular mechanics approach," *Smart Structures and Systems* **13**(4), 685–709 (2014).

[17] Eberhardt, O. and Wallmersperger, T., "Energy consistent modified molecular structural mechanics model for the determination of the elastic properties of single wall carbon nanotubes," *Carbon* **95**, 166–180 (2015).

[18] Xia, Z., Wang, C., and Tan, H., "Elastic properties of graphene: A pseudo-beam model with modified internal bending moment and its application," *Physica E: Low-dimensional Systems and Nanostructures* **98**, 45 – 52 (2018).

[19] Brenner, D. W., Shenderova, O. A., Harrison, J. A., Stuart, S. J., Ni, B., and Sinnott, S. B., "A second-generation reactive empirical bond order (rebo) potential energy expression for hydrocarbons," *Journal of Physics: Condesed Matter* **14**, 783–802 (2002).